136b Structure, Stability and Electronic Properties of Silicon Nanowires [Invited]

Madhu Menon

We present our results for the structural and electronic properties of various types of Si-nanowires. The nanowires investigated include, tetrahedral, clathrate and polycrystalline types. The tetrahedral nanowires are found to be the most stable. The small diameter nanowires show direct band-gaps indicating quantum confinement, while the larger diameter nanowires show indirect band-gaps. We show that a full coverage with H results in clathrate-like behavior for these nanowires, while a partial coverage results in amorphous-like behavior. The band gap vs. diameter dependence as well as the transport properties of bare nanowires are found to differ significantly from those for H-saturated nanowires. This indicates the tremendous potential for these nanowires in sensor applications.